Supporting Information

A Combined Experimental and Computational Investigation on the Unusual Molecular Mechanism of the Lossen Rearrangement Reaction Activated by Carcinogenic Halogenated Quinones

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CONTENTS

1. Analysis of the reaction products of 2,5-DCBQ/BHA. The reaction of 2,5-DCBQ with BHA was firstly studied by electrospray ionization mass spectrometry (ESI-MS), since ESI is considered as a soft ionization mode for facile obtaining of the molecular ions.[1] A small portion (20 μl) of reaction solution of 1 mM 2,5-DCBQ with 1, 2, or 4 mM BHA in 1 ml Chelex-treated CH_3COONH_4 buffer at room temperature during the reaction period of 0-30 min were directly injected into MS. All other experimental parameters of MS are the same as described previously in ref. 2. The direct MS spectra of the reaction products of 2,5-DCBQ/BHA are shown in Fig. S1.

2. NMR identification of P_1 and P_2. The ^{1}H-NMR and ^{13}C-NMR spectra for P_1 and P_2 using tetramethylsilane ($(CH_3)_4Si$) as internal standard and DMSO-d_6 as solvent were shown in Fig. S2 and S3, respectively, and the NMR assignments with chemical shifts were shown in Table S1. P_1 or P_2 was identified by ^{1}H- and ^{13}C-NMR as the single- and double-substituted 2,5-DCBQ adducts with BHA, respectively (Fig. S2, Fig. S3, Table S1). The singlet line at δ = 12.85 in ^{1}H-NMR and the line at δ = 165.8 in ^{13}C-NMR were assigned to the N-H proton and C=O carbon of -C(O)-NH-O- of P_1, respectively. Similarly, the singlet line at δ = 12.85 in ^{1}H-NMR and the line at δ = 165.5 in ^{13}C-NMR were assigned to the N-H proton and C=O carbon of -C(O)-NH-O- of P_2, respectively. This assignment is in agreement with the previously reported NMR data for similar *O*-substituted benzohydroxamate compounds.[3-6]

3. Direct detection and identification of phenyl isocyanate from P_1 via pyrolysis by GC/MS. Preliminary experiment showed that the solid form of P_1 decomposed at its

melting point (146.3 ℃), so pyrolysis of solid P_1 was performed for direct detection of phenyl isocyanate in GC/MS. Gas chromatography-mass spectrometry (GC/MS) was performed with a nonpolar capillary column (0.25 mm×30 m). 2 μl n-hexane containing P_1 (2 mg/ml) was injected to GC/MS. The injector was set at 250 ℃, and the oven temperature was programmed at 50 ℃ for 2 min, ramped at 5 ℃/min to 280 ℃, and maintained at this temperature for 10 min. The carrier gas was helium with a constant flow rate of 1.0 ml/min. The mass spectrometer was operated in the electron impact ionization mode at 70 eV with an interface temperature of 280 ℃ and a source temperature of 230 ℃. Positive fragment ions were analyzed over mass range (50-500 *m/z*) in the scan mode. Reagent-grade phenyl isocyanate was using as standard reference to identification of the pyrolysis product of P_1.

4. Analysis of the reaction products of other C_nBQ/BHA by HPLC/MS. The reactions of 2-chloro (2-CBQ), 2,6-dichloro (2,6-DCBQ), 2,3-dichloro (2,3-DCBQ), 2,3,5-trichloro (TrCBQ) -1,4-benzoquinone with BHA were performed as that of 2,5-DCBQ/BHA: 1 mM C_nBQ was mixed with 1 mM BHA in 1 ml Chelex-treated CH_3COONH_4 buffer (100 mM, pH 7.0) at room temperature for 1 min and then was injected into HPLC/MS.

For detection of the products of 2-CBQ, 2,6-DCBQ, 2,3-DCBQ with BHA, the experimental conditions of HPLC/MS were as that of 2,5-DCBQ/BHA described in methods. The HPLC/MS profiles are shown in Fig. S4. The main product of 2,6-DCBQ/BHA was eluted at 5.91 min and showed the molecular ion peak $[M-H]^-$ at *m/z* 276, and the fragment ion at *m/z* 157, both of which were one chlorine isotope peak

clusters, suggesting it was the 1:1 adduct of 2,6-DCBQ with BHA, just as similar as P_1 in 2,5-DBQQ/BHA. The main product of 2,3-DCBQ/BHA was 2-chloro-3-hydroxy-1,4-benzoquinone, not the 1:1 2,3-DCBQ/BHA adduct, which was isolated with the elute time of 2.41 min and showed the molecular ion peak $[M-H]^-$ at *m/z* 157. The main product peak of 2-CBQ/BHA was appeared at 4.91 min, and showed that the molecular ion peak $[M-H]^-$ at *m/z* 242, and the fragment ion at *m/z* 123, suggesting it is the 1:1 2-CBQ/BHA adduct.

For detection of the products of TrCBQ with BHA, the HPLC mobile phase were adjusted to a gradient elution by varying the proportion of 50 mM acetic acid (solvent A) to acetonitrile (solvent B) at a rate of 1.0 ml/min: the mobile phase composition started at 15% B in 5 min, then followed by a linear increase of B to 50% within 1 min, then 50% B for 12 min, and then followed by a linear decrease of B to 15% within 1 min, then 15% B for 8 min. All other analytic parameters was the same as that of 2,5-DCBQ/BHA. Besides by MS analysis, the reaction products of TrCBQ/BHA (1:1) were shown in Fig. S5 and determined by comparison with the typical products of C_nBQs/H_2O_2; the reaction conditions of C_nBQs/H_2O_2 were the same as described in our previous study,[7] in which we found that hydroxyl radicals were rapidly generated in a metal-independent way from C_nBQ/H_2O_2. For 2,5-DCBQ, 2,6-DCBQ, or 2,3-DCBQ)/H_2O_2, we also found that hydroxyl radicals generated were able to directly attack at the quinoid rings, resulting in formation of by-products 2,5-dichloro-3-hydroxy-1,4-benzoquinone (**6**) (eluted at 3.3 min, Fig. S5 A), 2,6-dichloro-3-hydroxy-1,4-benzoquinone (**7**) (eluted at 3.3 min, Fig. S5-A),

2,3-dichloro-5-hydroxy-1,4-benzoquinone (**5**) (eluted at 9.3 min, Fig. S5 A), respectively. All of the byproducts are two chlorine isotope peak clusters and showed the molecular ion peak $[M-H]^-$ at *m/z* 191.

In Fig. S5 A, two product peaks appeared from the reaction solution of TrCBQ/BHA (1:1): the one eluted at 3.2 min with molecular ion peak $[M-H]^-$ at *m/z* 191 might be **6** or **7**, the other, which was eluted at 15.26 min and showed that the molecular ion peak $[M-H]^-$ at *m/z* 310 and the fragment ion peak at *m/z* 191, both of which are two chlorine isotope peak clusters (Fig. S5 B), might be the relatively stable 1:1 TrCBQ/BHA adduct formed when 5-chloro of TrCBQ was substituted by BHA. It was further supported by the fact that its thermal decomposition led to formation of **5**, which was eluted at 9.3 min (Fig. S5-A) with the molecular ion peak $[M-H]^-$ at *m/z* 191 (Fig. S5 C).

5. Experimental measurement of pK_a values of P_1 and hydroxylated chloroquinoid products in solution. The pK_a value of P_1 was measured by the titration method with a pH meter.[8] The pK_a values of some easily prepared hydroxylated chlorobenzoquinones were also obtained by experimental measurement: 2-chloro-3-hydroxy-1,4-benzoquinone (**2**) was directly collected by semi-preparative HPLC from the reaction solution of 2,3-DCBQ/BHA (1:1). 2-chloro-5-hydroxy-1,4-benzoquinone (**3**) was collected by semi-preparative HPLC from the thermal decomposition of P_1 in buffer solution (pH 7.0, 50 ℃). Their pK_a values were measured with a UV-visible spectrophotometer.

6. SI Figures and Tables

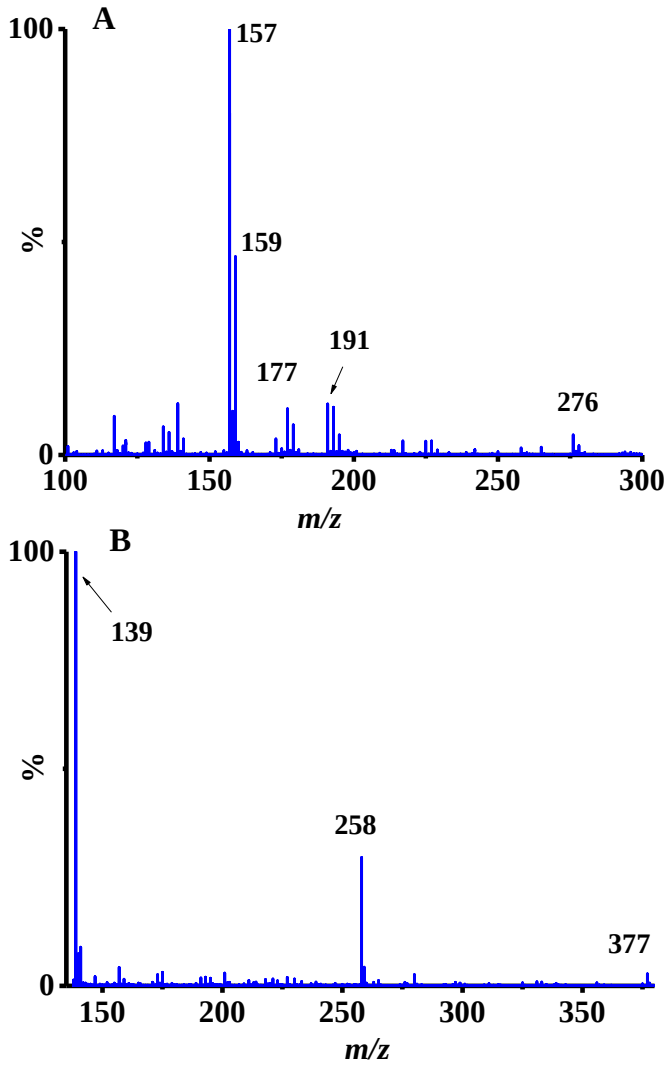


Fig. S1: Mass spectra of the reaction solutions of 2,5-DCBQ/BHA (A 1:1, B 1:2) in CH_3COONH_4 buffer (pH 7.0, 0.1 M) at room temperature.

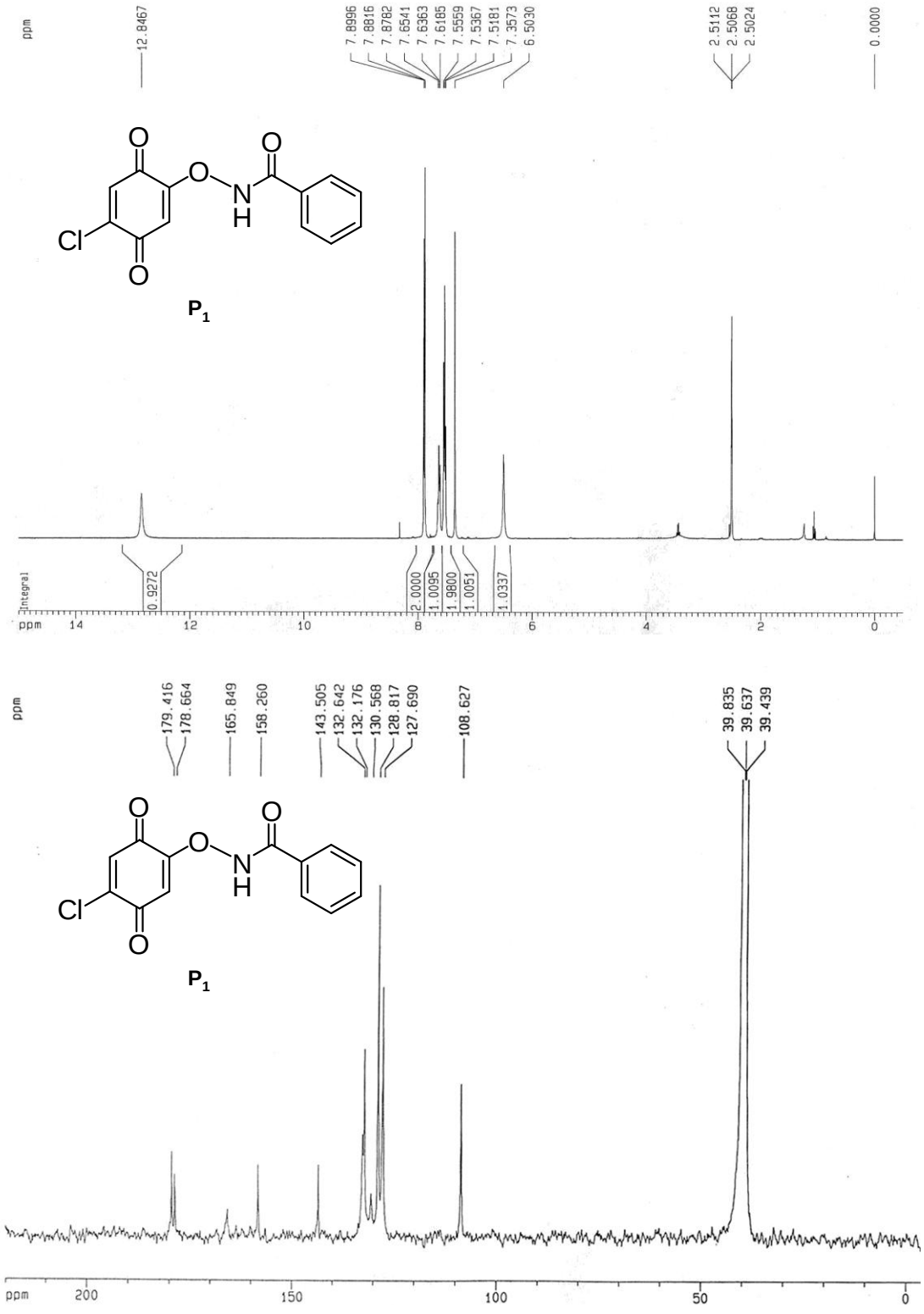


Fig. S2: The ^{1}H-NMR and ^{13}C-NMR of P_1 in DMSO-d_6.

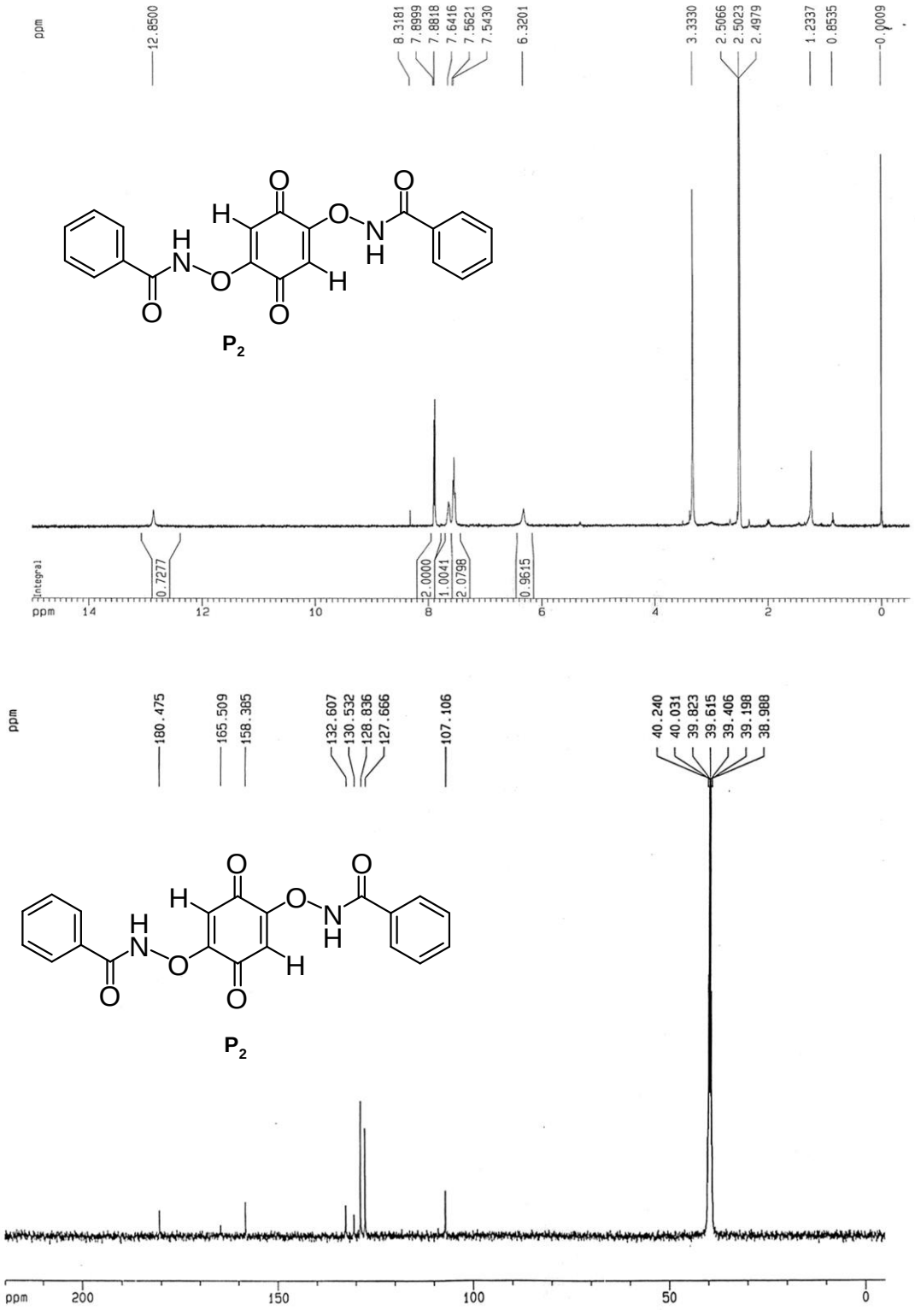


Fig. S3: The ^{1}H-NMR and ^{13}C-NMR of P_2 in DMSO-d_6.

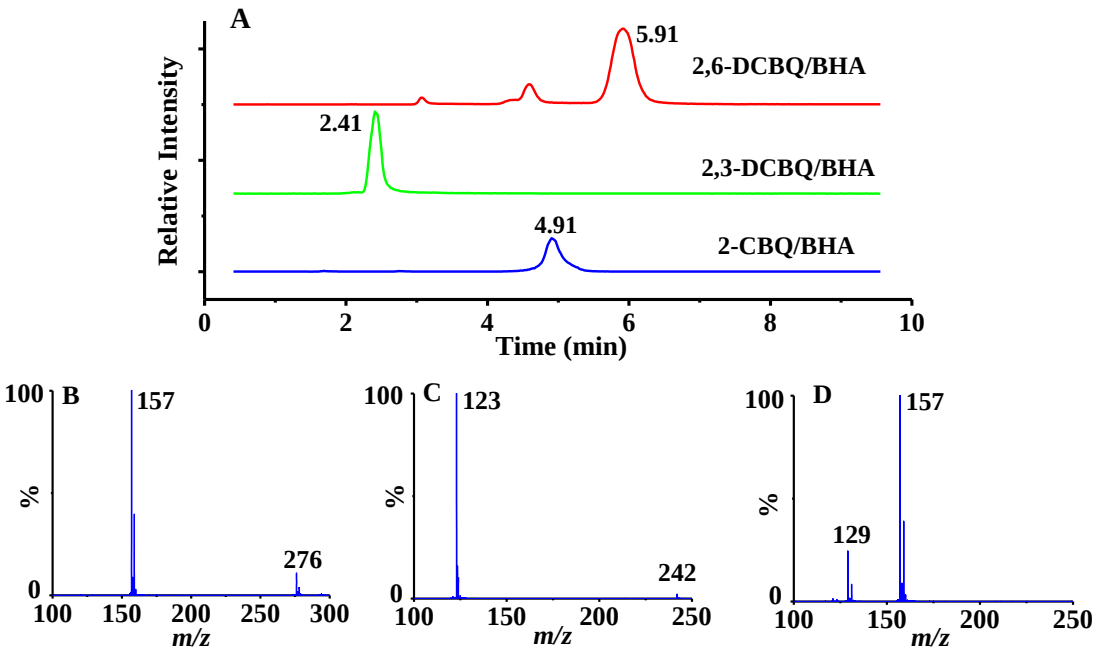


Fig. S4: (A) The HPLC/MS selected ion monitoring (SIM）profile of the reaction mixtures of BHA with 2,6-DCBQ (monitoring at *m/z* 157, the fragment ion peak, corresponding to the anion of 2-chloro-6-hydroxy-1,4-benzoquinone (**4**)), and 2,3-DCBQ (monitoring at *m/z* 157, the fragment ion peak, corresponding to the anion of 2-chloro-3-hydroxy-1,4-benzoquinone (**2**)). 2-CBQ (monitoring at *m/z* 123, the fragment ion peak, corresponding to the anion of 2-hydroxy-1,4-benzoquinone(**1**)). Other experimental conditions were just the same as the reaction of 2,5-DCBQ/BHA. (B) The MS spectrum of the product peak at the retention time of 5.91 min in the HPLC/MS chromatogram of 2,6-DCBQ/BHA, showing the main product of 2,6-DCBQ/BHA was the 1:1 adduct of 2,6-DCBQ with BHA; (C) The MS spectrum of the product peak at the retention time of 4.91 min in the HPLC/MS chromatogram of 2-CBQ/BHA, showing the main product of 2-CBQ/BHA was the 1:1 adduct of 2-CBQ with BHA; (D) The MS spectrum of the product peak at the retention time of 2.41 min in the HPLC/MS chromatogram of 2,3-DCBQ/BHA, showing the main product of 2,3-DCBQ/BHA was 2-chloro-3-hydroxy-1,4-benzoquinone.

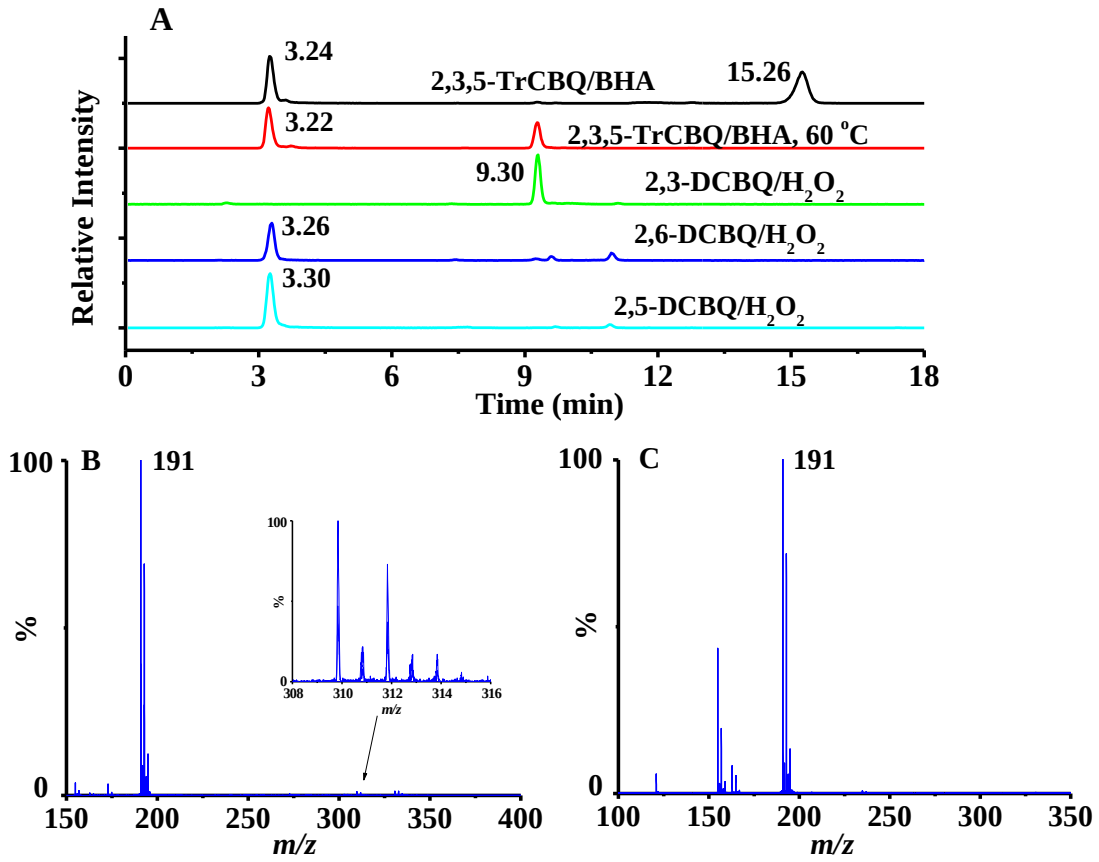
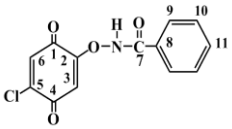


Fig. S5: (A) The HPLC/MS selected ion monitoring (SIM) profile of the 1:1 reaction mixtures of 2,3,5-TrCBQ/BHA (1:1), 2,3,5-TrCBQ/BHA (1:1, 60 ℃), 2,3-DCBQ /H_2O_2 (1:10), 2,6-DCBQ/H_2O_2 (1:10), 2,5-DCBQ/H_2O_2 (1:10), which were all monitored at *m/z* 191, corresponding to dichloro-hydroxyl-1,4-benzoquinone. The reactions were performed at room temperature, except for the thermal reaction of 2,3,5-TrCBQ/BHA (1:1, 60 ℃). (B) The MS spectrum of the product peak at the retention time of 15.26 min in the HPLC/MS chromatogram of 2,3,5-TrCBQ/BHA; (C) The MS spectrum of the product peak at the retention time of 9.30 min in the HPLC/MS chromatogram of 2,3,5-TrCBQ/BHA (1:1, 60 ℃) or 2,3-DCBQ/BHA.

Table S1: NMR (DMSO-d_6) assignments for $\mathbf{P_1}$ (A) and $\mathbf{P_2}$ (B)

A

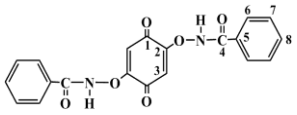
Formula of P_1



δ_H (ppm)	position	δ_C (ppm)	position
12.85（s, 1H）	N-H	179.4, 178.7	C-1,4
7.88（m, 2H）	C-10	165.8	C-7
7.64（m, 1H）	C-11	158.3, 143.5	C-2,5
7.54（m, 2H）	C-9	132.6	C-11
7.36（s, 1H）	C-6	130.6	C-8
6.50（s, 1H）	C-3	128.8, 127.7	C-9,10

B

Formula of P_2



δ_H (ppm)	position	δ_C (ppm)	position
12.85（s, 2H）	N-H	C-1	180.5
7.89（m, 4H）	C-7	C-4	165.5
7.64（m, 2H）	C-8	C-2	158.4
7.55（m, 4H）	C-6	C-5	132.6
6.32（s, 2H）	C-3	C-8	130.5
		C-6,7	128.8, 127.7

Table S2: Calculated and measured pK_a values of a series of hydroxylated benzoquinones

No.	Hydroxylated benzoquinones	Formula	pK_a	
			expt.	calc.
1	2-hydroxy-		4.0-4.2[a]	4.23
2	2-chloro-3-hydroxy-		2.28[b]	2.56
3	2-chloro-5-hydroxy-		3.63[b]	3.56
4	2-chloro-6-hydroxy-		-	3.65
5	2,3-dichloro-5-hydroxy-		-	2.89
6	2,5-dichloro-3-hydroxy-		-	1.88
7	2,6-dichloro-3-hydroxy-		1.57[c]	1.68
8	2,3,5-trichloro-6-hydroxy-		1.09[d]	1.04
9	2,5-dichloro-3,6-dihydroxy-		0.58[e], 0.76[f] (pK_{a1}) 2.58[f], 3.18[e] (pK_{a2})	0.82 2.33

[a] ref. 9-11 [b] measured in this work. [c] ref. 12. [d] ref. 13. [e] ref. 14. [f] ref. 15

Table S3: The activation energies of the reactions of C_nBQ/BHA (1:1)

ΔG（kcal/mol）	**TCBQ**	**TrCBQ-2**	**TrCBQ-3**	**TrCBQ-5**	**2,3-DCBQ**	**2,5-DCBQ**	**2,6-DCBQ**	**CBQ**
S_N2(1)	5.79	7.12	7.68	8.59	9.64	10.14	10.62	12.66
LR(1)	16.97	17.90	18.01	22.89	17.64	23.90	23.93	24.43

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Cartesian coordinate of some key structures and IRC calculations for TS in Fig. 4

TCBQ in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.281337	-0.676229	0.000337
2	6	0	-1.281337	0.676229	0.000256
3	6	0	0.000000	1.457326	0.000616
4	6	0	1.281337	0.676229	0.000255
5	6	0	1.281337	-0.676229	0.000338
6	6	0	0.000000	-1.457326	0.001044
7	8	0	0.000000	-2.671841	-0.000243
8	8	0	0.000000	2.671841	0.000263
9	17	0	2.721754	-1.616912	-0.000194
10	17	0	2.721753	1.616913	-0.000313
11	17	0	-2.721753	-1.616913	-0.000197
12	17	0	-2.721754	1.616912	-0.000310

Zero-point correction= 0.046899 (Hartree/Particle)
Thermal correction to Energy= 0.057936
Thermal correction to Enthalpy= 0.058880
Thermal correction to Gibbs Free Energy= 0.007774
Sum of electronic and zero-point Energies= -2219.781947
Sum of electronic and thermal Energies= -2219.770909
Sum of electronic and thermal Enthalpies= -2219.769965
Sum of electronic and thermal Free Energies= -2219.821071

BHA^- in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.458195	-0.672466	-0.203230
2	7	0	-2.134251	-0.646292	-0.174756
3	6	0	-1.337235	0.407802	0.101579
4	8	0	-1.730324	1.573333	0.354096

5	6	0	0.136155	0.099581	0.045049
6	6	0	1.009220	1.192054	-0.138835
7	6	0	2.390955	1.015770	-0.203584
8	6	0	2.954097	-0.260023	-0.072073
9	6	0	2.104600	-1.353403	0.139670
10	6	0	0.721052	-1.175638	0.206605
11	1	0	-1.669656	-1.507628	-0.456657
12	1	0	0.556752	2.175278	-0.219670
13	1	0	3.036249	1.879429	-0.353943
14	1	0	4.031860	-0.398139	-0.115414
15	1	0	2.522935	-2.349344	0.272303
16	1	0	0.096706	-2.039347	0.419283

Zero-point correction= 0.117663 (Hartree/Particle)
Thermal correction to Energy= 0.125929
Thermal correction to Enthalpy= 0.126874
Thermal correction to Gibbs Free Energy= 0.083960
Sum of electronic and zero-point Energies= -475.458681
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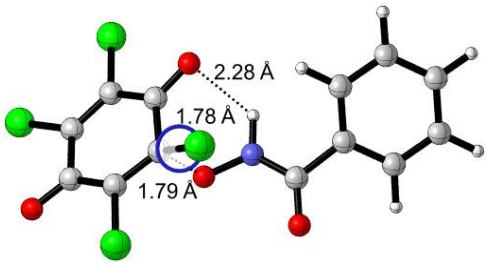
Sum of electronic and thermal Enthalpies= -475.449470
Sum of electronic and thermal Free Energies= -475.492383

TS_1 in Fig. 4A



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.181338	-1.425628	0.126182
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3	6	0	3.185643	0.884122	-0.181584
4	6	0	1.968423	1.448701	0.280404
5	6	0	0.812675	0.682755	0.546919
6	6	0	0.941579	-0.825279	0.664299

7	8	0	0.035161	-1.513831	1.118725
8	8	0	4.208105	1.504127	-0.513928
9	8	0	-0.103266	0.527184	-0.986480
10	7	0	-1.353696	0.027344	-0.857117
11	6	0	-2.483482	0.800648	-0.864236
12	8	0	-2.527141	1.976865	-1.214411
13	6	0	-3.732056	0.042257	-0.475562
14	6	0	-4.939973	0.418858	-1.080747
15	6	0	-6.130868	-0.224765	-0.745245
16	6	0	-6.132286	-1.243056	0.215165
17	6	0	-4.936380	-1.607564	0.838975
18	6	0	-3.739754	-0.970311	0.497039
19	1	0	-1.399103	-0.943728	-0.563717
20	1	0	-4.921755	1.226138	-1.806013
21	1	0	-7.059469	0.069811	-1.227454
22	1	0	-7.060883	-1.741242	0.481717
23	1	0	-4.932314	-2.382570	1.600729
24	1	0	-2.822852	-1.239262	1.014123
25	17	0	-0.372897	1.336805	1.698747
26	17	0	4.701199	-1.319082	-0.822314
27	17	0	1.882664	3.201994	0.314429
28	17	0	2.230028	-3.171391	0.091361

Zero-point correction= 0.165977 (Hartree/Particle)
Thermal correction to Energy= 0.186098
Thermal correction to Enthalpy= 0.187042
Thermal correction to Gibbs Free Energy= 0.114212
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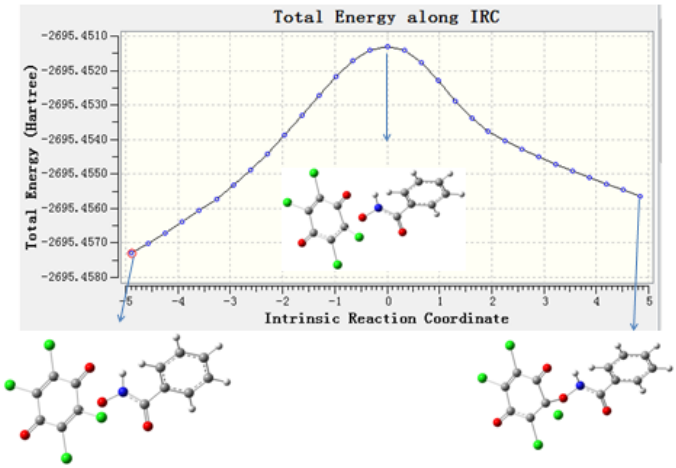
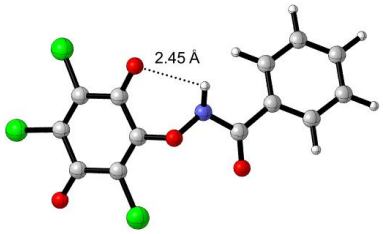
The IRC computational result of TS_1 in Fig. 4A:



IN_1 in Fig. 4A

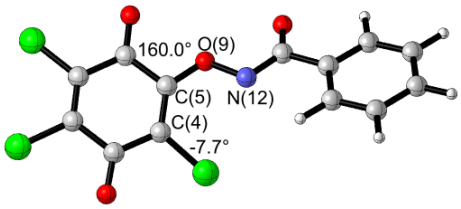


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.481248	-1.269642	0.162686
2	6	0	3.338962	-0.328319	-0.292536
3	6	0	2.979048	1.135478	-0.277548
4	6	0	1.610727	1.499453	0.200739
5	6	0	0.742918	0.549565	0.619982
6	6	0	1.152285	-0.883216	0.731429
7	8	0	0.433465	-1.695299	1.290638
8	8	0	3.767459	1.975962	-0.661850
9	8	0	-0.466064	0.905050	1.133988
10	17	0	1.204378	3.167660	0.182577
11	17	0	2.842590	-2.953691	0.179232
12	7	0	-1.531184	0.109838	0.639248
13	6	0	-2.577365	0.858619	0.082865
14	8	0	-2.462595	2.031812	-0.218845
15	6	0	-3.823082	0.056433	-0.152535

16	6	0	-5.025958	0.766489	-0.282801
17	6	0	-6.221543	0.083796	-0.501108
18	6	0	-6.224602	-1.311336	-0.601515
19	6	0	-5.026912	-2.022371	-0.487418
20	6	0	-3.827657	-1.343613	-0.262690
21	1	0	-1.755788	-0.602229	1.327048
22	1	0	-5.002236	1.848835	-0.213155
23	1	0	-7.150110	0.638738	-0.595464
24	1	0	-7.156163	-1.841913	-0.775389
25	1	0	-5.023475	-3.104045	-0.582028
26	1	0	-2.899762	-1.904903	-0.208460
27	17	0	4.897695	-0.701708	-0.915694

Zero-point correction= 0.167633 (Hartree/Particle)
Thermal correction to Energy= 0.186375
Thermal correction to Enthalpy= 0.187319
Thermal correction to Gibbs Free Energy= 0.116433
Sum of electronic and zero-point Energies= -2235.002457
Sum of electronic and thermal Energies= -2234.983715
Sum of electronic and thermal Enthalpies= -2234.982771
Sum of electronic and thermal Free Energies= -2235.053657

IN_2 in Fig. 4A

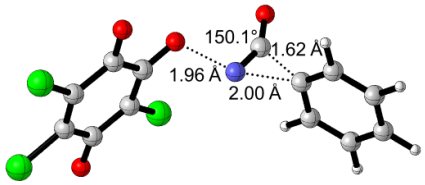


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.232362	-0.828416	0.137016
2	6	0	3.455388	0.500700	0.105525
3	6	0	2.345188	1.499054	-0.134345
4	6	0	0.996906	0.972817	-0.276886
5	6	0	0.722164	-0.380373	-0.168286
6	6	0	1.847714	-1.373892	0.015429
7	8	0	1.640438	-2.572595	0.090952
8	8	0	2.633393	2.693440	-0.222636

9	8	0	-0.420045	-1.028628	-0.210177
10	17	0	-0.188817	2.183441	-0.702523
11	17	0	4.492070	-2.005354	0.350843
12	7	0	-1.612659	-0.298788	0.056114
13	6	0	-2.658354	-1.069495	-0.321566
14	8	0	-2.656405	-2.176308	-0.892817
15	6	0	-3.976172	-0.399516	0.033298
16	6	0	-5.158540	-1.097591	-0.248527
17	6	0	-6.404667	-0.542026	0.051639
18	6	0	-6.486197	0.725500	0.637144
19	6	0	-5.310302	1.430514	0.918505
20	6	0	-4.064290	0.873940	0.620441
21	1	0	-5.067504	-2.077770	-0.705905
22	1	0	-7.312719	-1.097399	-0.172304
23	1	0	-7.455070	1.160976	0.870389
24	1	0	-5.363809	2.418253	1.370526
25	1	0	-3.150889	1.417628	0.834478
26	17	0	5.038650	1.179281	0.297040

Zero-point correction= 0.153498 (Hartree/Particle)
Thermal correction to Energy= 0.172101
Thermal correction to Enthalpy= 0.173046
Thermal correction to Gibbs Free Energy= 0.102453
Sum of electronic and zero-point Energies= -2234.496676
Sum of electronic and thermal Energies= -2234.478072
Sum of electronic and thermal Enthalpies= -2234.477128
Sum of electronic and thermal Free Energies= -2234.547721

TS_2 in Fig. 4A

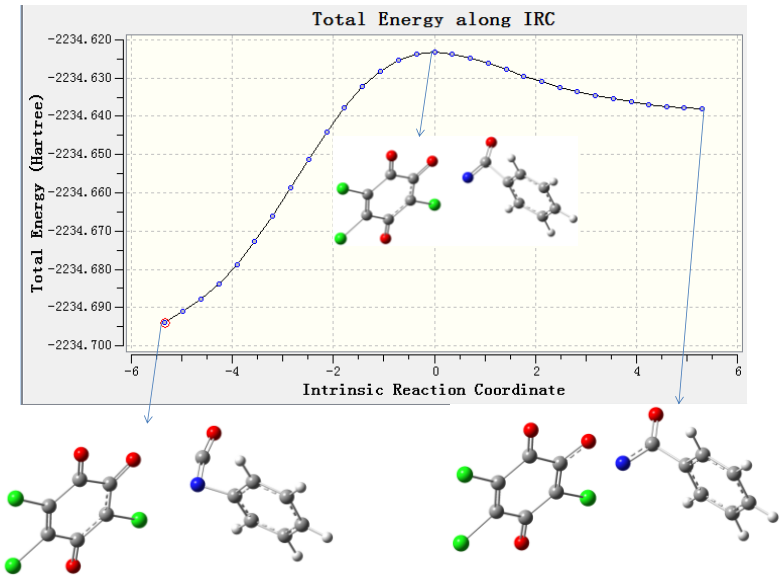


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.880742	-0.492009	0.381523
2	6	0	2.844711	-0.463398	1.220802

3	8	0	3.248599	-0.508083	2.375788
4	6	0	3.821062	-0.286831	-0.055483
5	8	0	0.248377	-0.831479	1.418887
6	6	0	-0.788399	-0.347073	0.875778
7	6	0	4.212279	0.999826	-0.445131
8	6	0	5.276391	1.159295	-1.334931
9	6	0	5.937568	0.037318	-1.847838
10	6	0	5.529462	-1.247922	-1.471578
11	6	0	4.465584	-1.412427	-0.582838
12	6	0	-1.063183	0.995141	0.613388
13	6	0	-2.262975	1.474200	-0.023034
14	6	0	-3.293020	0.420041	-0.418553
15	6	0	-3.117782	-0.892131	-0.171657
16	6	0	-1.863803	-1.380933	0.487784
17	17	0	0.082831	2.218693	1.111980
18	8	0	-2.520232	2.657026	-0.256158
19	17	0	-4.292878	-2.110240	-0.584872
20	8	0	-1.697723	-2.565271	0.705858
21	1	0	3.680061	1.859632	-0.050819
22	1	0	5.583215	2.157352	-1.636963
23	1	0	6.761438	0.163436	-2.545518
24	1	0	6.034250	-2.120364	-1.878705
25	1	0	4.130810	-2.403337	-0.291687
26	17	0	-4.717865	1.035027	-1.191945

Zero-point correction= 0.149664 (Hartree/Particle)
Thermal correction to Energy= 0.169011
Thermal correction to Enthalpy= 0.169956
Thermal correction to Gibbs Free Energy= 0.096697
Sum of electronic and zero-point Energies= -2234.473611
Sum of electronic and thermal Energies= -2234.454264
Sum of electronic and thermal Enthalpies= -2234.453320
Sum of electronic and thermal Free Energies= -2234.526578

The IRC computational result on TS_2 in Fig. 4A



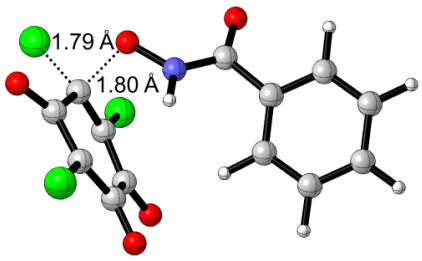
TrCBQO$^-$ in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.242279	0.487174	0.000004
2	6	0	0.806260	-0.788531	0.000061
3	6	0	-0.678831	-1.175532	0.000198
4	6	0	-1.597480	-0.092850	0.000066
5	6	0	-1.258273	1.282519	-0.000002
6	6	0	0.265240	1.616885	-0.000078
7	8	0	0.643967	2.773547	0.000026
8	8	0	-0.957021	-2.384791	-0.000175
9	8	0	-2.035530	2.247842	-0.000017
10	17	0	-3.309692	-0.507266	0.000020
11	17	0	2.936309	0.926574	-0.000045
12	17	0	1.909471	-2.129353	0.000015

Zero-point correction= 0.047741 (Hartree/Particle)
Thermal correction to Energy= 0.058593
Thermal correction to Enthalpy= 0.059537
Thermal correction to Gibbs Free Energy= 0.009130
Sum of electronic and zero-point Energies= -1834.919519
Sum of electronic and thermal Energies= -1834.908667
Sum of electronic and thermal Enthalpies= -1834.907723

Sum of electronic and thermal Free Energies= -1834.958130

TS_3 in Fig. 4A



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.467762	-0.606199	-1.134591
2	6	0	1.591018	-1.341977	-0.965612
3	8	0	1.702659	-2.553475	-1.194419
4	6	0	2.796321	-0.526321	-0.538113
5	8	0	-0.731492	-1.126271	-1.480234
6	6	0	-1.945177	-0.675055	-0.228384
7	6	0	2.727092	0.559449	0.349781
8	6	0	3.891472	1.242747	0.716304
9	6	0	5.133792	0.852348	0.209554
10	6	0	5.210571	-0.241905	-0.661598
11	6	0	4.051224	-0.928713	-1.022935
12	6	0	-1.440357	-0.784902	1.085091
13	6	0	-0.804135	0.292751	1.762105
14	6	0	-0.809048	1.694336	1.050302
15	6	0	-1.516320	1.787774	-0.178805
16	6	0	-2.267565	0.740481	-0.781516
17	17	0	-1.320801	-2.384682	1.859546
18	8	0	-0.240490	0.214400	2.868472
19	17	0	-1.679035	3.410021	-0.910274
20	8	0	-3.071364	0.864019	-1.717796
21	1	0	1.784580	0.866878	0.791672
22	1	0	3.814214	2.075292	1.410162
23	1	0	6.036346	1.387695	0.497965
24	1	0	6.174496	-0.561005	-1.054044
25	1	0	4.090543	-1.794881	-1.676632
26	1	0	0.484056	0.406646	-1.036926

27	17	0	-3.181768	-1.869823	-0.738050
28	8	0	-0.194893	2.625441	1.604246

IN_3 in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.214343	-0.483740	0.157892
2	6	0	2.375974	-1.133801	-0.148449
3	8	0	2.457421	-2.313582	-0.481494
4	6	0	3.602851	-0.265309	0.019311
5	8	0	0.050167	-1.244777	-0.118761
6	6	0	-1.132698	-0.587732	-0.028551
7	6	0	3.581391	1.024165	0.574493
8	6	0	4.762783	1.760843	0.685693
9	6	0	5.975276	1.220382	0.247761
10	6	0	6.001920	-0.065225	-0.302075
11	6	0	4.823059	-0.802923	-0.413644
12	6	0	-2.248393	-1.360722	0.085918
13	6	0	-3.589700	-0.767606	0.124161
14	6	0	-3.701068	0.791548	0.031199
15	6	0	-2.474039	1.514309	-0.104911
16	6	0	-1.206173	0.927407	-0.159772
17	17	0	-2.127789	-3.100746	0.192473
18	8	0	-4.604505	-1.436650	0.234299
19	17	0	-2.565891	3.263684	-0.237250
20	8	0	-0.117791	1.567145	-0.319319
21	1	0	2.652524	1.458271	0.929509
22	1	0	4.733316	2.757804	1.116421
23	1	0	6.892502	1.796791	0.335599
24	1	0	6.940862	-0.492562	-0.644066
25	1	0	4.819084	-1.803890	-0.832291
26	8	0	-4.829188	1.283063	0.079164
27	1	0	0.977929	0.526215	-0.067141

Zero-point correction= 0.167690 (Hartree/Particle)
Thermal correction to Energy= 0.186039
Thermal correction to Enthalpy= 0.186984

Thermal correction to Gibbs Free Energy=	0.117389
Sum of electronic and zero-point Energies=	-1850.151454
Sum of electronic and thermal Energies=	-1850.133105
Sum of electronic and thermal Enthalpies=	-1850.132161
Sum of electronic and thermal Free Energies=	-1850.201756

TS_{1a} in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.287439	1.314076	-0.523896
2	6	0	-3.560349	1.244626	-0.081170
3	6	0	-4.239446	-0.073432	0.164878
4	6	0	-3.405646	-1.277366	0.022185
5	6	0	-2.099317	-1.226067	-0.362858
6	6	0	-1.525053	0.070883	-0.867687
7	8	0	-0.596416	0.101043	-1.665299
8	8	0	-5.414414	-0.115951	0.507064
9	8	0	-1.391667	-2.358152	-0.455717
10	7	0	-0.038692	-2.225082	0.001366
11	6	0	0.788940	-3.116930	-0.585918
12	8	0	0.471281	-3.933747	-1.458484
13	6	0	2.206869	-3.059521	-0.052639
14	6	0	3.185903	-3.745151	-0.786317
15	6	0	4.515585	-3.752812	-0.363236
16	6	0	4.883411	-3.077721	0.805557
17	6	0	3.911635	-2.398142	1.545634
18	6	0	2.579665	-2.388149	1.122736
19	1	0	0.104939	-1.201281	0.612681
20	1	0	2.873102	-4.270739	-1.682635
21	1	0	5.264488	-4.285833	-0.943801
22	1	0	5.918554	-3.081843	1.137675
23	1	0	4.186594	-1.871713	2.455489
24	1	0	1.839483	-1.858289	1.712684
25	17	0	-4.524927	2.651125	0.226255
26	8	0	0.033906	-0.028606	1.146819
27	7	0	1.058256	0.678559	0.584827
28	6	0	1.601503	1.758474	1.210840
29	8	0	1.326557	2.117368	2.358179

30	6	0	2.639217	2.487399	0.388081
31	6	0	2.854393	3.843052	0.677489
32	6	0	3.800801	4.580149	-0.034733
33	6	0	4.557689	3.967885	-1.039638
34	6	0	4.363279	2.612987	-1.321368
35	6	0	3.411666	1.875367	-0.611837
36	1	0	1.096291	0.614089	-0.432553
37	1	0	2.269501	4.295095	1.471980
38	1	0	3.950615	5.631994	0.195131
39	1	0	5.298058	4.540041	-1.592735
40	1	0	4.958355	2.123934	-2.087917
41	1	0	3.294125	0.816754	-0.822218
42	17	0	-4.152376	-2.791187	0.438780
43	17	0	-1.482983	2.803601	-0.866461

Zero-point correction=	0.282428 (Hartree/Particle)
Thermal correction to Energy=	0.310644
Thermal correction to Enthalpy=	0.311589
Thermal correction to Gibbs Free Energy=	0.217744
Sum of electronic and zero-point Energies=	-2710.526341
Sum of electronic and thermal Energies=	-2710.498124
Sum of electronic and thermal Enthalpies=	-2710.497180
Sum of electronic and thermal Free Energies=	-2710.591025

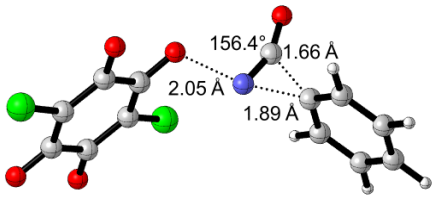
IN_4 in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.286906	-0.419669	0.122743
2	6	0	-2.307966	-1.038603	-0.469895
3	8	0	-2.342661	-1.961785	-1.322352
4	6	0	-3.630245	-0.457510	0.030346
5	8	0	-0.050591	-1.053713	-0.281989
6	6	0	1.049720	-0.325611	-0.193261
7	6	0	-3.723810	0.646467	0.896973
8	6	0	-4.970019	1.127418	1.306153
9	6	0	-6.150513	0.516477	0.860971
10	6	0	-6.065913	-0.579928	-0.003703
11	6	0	-4.817470	-1.057247	-0.415419

12	6	0	1.204320	1.033907	-0.323886
13	6	0	2.500384	1.684253	-0.135805
14	6	0	3.750689	0.804243	0.202106
15	6	0	3.531472	-0.589643	0.227774
16	6	0	2.277701	-1.239025	0.052131
17	17	0	-0.091460	2.120719	-0.845844
18	8	0	2.657284	2.898733	-0.249364
19	17	0	4.934084	-1.636207	0.542683
20	8	0	2.086916	-2.464268	0.097720
21	1	0	-2.805961	1.116422	1.232975
22	1	0	-5.021803	1.986041	1.973570
23	1	0	-7.120296	0.893446	1.181480
24	1	0	-6.974895	-1.062906	-0.360004
25	1	0	-4.719159	-1.901489	-1.091598
26	8	0	4.828520	1.395815	0.399885

Zero-point correction= 0.154554 (Hartree/Particle)
Thermal correction to Energy= 0.172868
Thermal correction to Enthalpy= 0.173812
Thermal correction to Gibbs Free Energy= 0.104145
Sum of electronic and zero-point Energies= -1849.527451
Sum of electronic and thermal Energies= -1849.509137
Sum of electronic and thermal Enthalpies= -1849.508192
Sum of electronic and thermal Free Energies= -1849.577860

TS_4 in Fig. 4A



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.684370	-0.487179	0.476246
2	6	0	2.571120	-0.489028	1.380006
3	8	0	3.006274	-0.520446	2.520248
4	6	0	3.511259	-0.373697	0.011595
5	8	0	-0.133635	-0.693115	1.404174

6	6	0	-1.126202	-0.211869	0.772161
7	6	0	3.953235	0.892262	-0.402091
8	6	0	5.016806	0.998689	-1.299550
9	6	0	5.640046	-0.153126	-1.797619
10	6	0	5.186352	-1.416359	-1.395342
11	6	0	4.122622	-1.528768	-0.498664
12	6	0	-1.305825	1.125325	0.414783
13	6	0	-2.451394	1.641447	-0.289427
14	6	0	-3.587653	0.628438	-0.683196
15	6	0	-3.388534	-0.717833	-0.296416
16	6	0	-2.253755	-1.235641	0.386944
17	17	0	-0.069148	2.314505	0.890279
18	8	0	-2.602164	2.831406	-0.591010
19	17	0	-4.680094	-1.882545	-0.711668
20	8	0	-2.079418	-2.423891	0.705036
21	1	0	3.443869	1.774709	-0.027466
22	1	0	5.352483	1.981538	-1.623235
23	1	0	6.463133	-0.067557	-2.503336
24	1	0	5.656629	-2.314286	-1.791067
25	1	0	3.750894	-2.502399	-0.193174
26	8	0	-4.572178	1.085534	-1.294813

DDBQO^{-2} in Fig. 4A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.430301	0.000493	0.000170
2	6	0	-0.789367	-1.265905	0.000093
3	6	0	0.790046	-1.266486	0.000421
4	6	0	1.430301	-0.000493	0.000164
5	6	0	0.789367	1.265905	0.000127
6	6	0	-0.790046	1.266486	0.000479
7	8	0	-1.363295	2.373656	-0.000138
8	8	0	1.363295	-2.373656	-0.000027
9	17	0	-3.229822	-0.000313	-0.000190
10	8	0	-1.363853	-2.372224	-0.000112
11	17	0	3.229821	0.000313	-0.000166
12	8	0	1.363854	2.372224	-0.000057

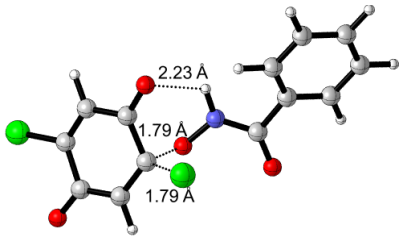
Zero-point correction=	0.049197 (Hartree/Particle)
Thermal correction to Energy=	0.059690
Thermal correction to Enthalpy=	0.060634
Thermal correction to Gibbs Free Energy=	0.011482
Sum of electronic and zero-point Energies=	-1449.918278
Sum of electronic and thermal Energies=	-1449.907785
Sum of electronic and thermal Enthalpies=	-1449.906841
Sum of electronic and thermal Free Energies=	-1449.955993

DCBQ in Fig. 4B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.413420	-0.269788	0.000183
2	6	0	-0.571430	-1.318678	0.000016
3	6	0	1.413356	0.269788	0.000026
4	6	0	0.571437	1.318708	0.000215
5	6	0	0.899085	-1.144492	0.000003
6	8	0	1.647538	-2.108044	0.000244
7	6	0	-0.899105	1.144511	0.000860
8	8	0	-1.647555	2.108051	-0.000226
9	17	0	-3.131229	-0.469432	-0.000218
10	17	0	3.131262	0.469408	-0.000242
11	1	0	-0.921924	-2.345037	-0.000269
12	1	0	0.921963	2.345082	0.000120

Zero-point correction=	0.065906 (Hartree/Particle)
Thermal correction to Energy=	0.074528
Thermal correction to Enthalpy=	0.075472
Thermal correction to Gibbs Free Energy=	0.030916
Sum of electronic and zero-point Energies=	-1300.591387
Sum of electronic and thermal Energies=	-1300.582764
Sum of electronic and thermal Enthalpies=	-1300.581820
Sum of electronic and thermal Free Energies=	-1300.626376

TS_1 in Fig. 4B1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.599426	1.452753	0.010493
2	6	0	-3.634514	0.631227	-0.245766
3	6	0	-3.612978	-0.871078	0.002650
4	6	0	-2.388185	-1.374555	0.503110
5	6	0	-1.234514	-0.583186	0.651511
6	6	0	-1.352360	0.924521	0.577820
7	8	0	-0.438925	1.682897	0.912161
8	8	0	-4.648809	-1.532655	-0.210844
9	8	0	-0.310034	-0.655353	-0.877080
10	7	0	0.946926	-0.145381	-0.809665
11	6	0	2.070487	-0.918015	-0.752008
12	8	0	2.113017	-2.124481	-0.989979
13	6	0	3.326264	-0.130962	-0.447829
14	6	0	4.528343	-0.569761	-1.022018
15	6	0	5.724716	0.097510	-0.759599
16	6	0	5.738377	1.203947	0.097656
17	6	0	4.548573	1.632384	0.692124
18	6	0	3.346733	0.970582	0.422529
19	1	0	0.990624	0.842566	-0.577350
20	1	0	4.500712	-1.443575	-1.665284
21	1	0	6.648243	-0.246897	-1.218264
22	1	0	6.671129	1.721212	0.307746
23	1	0	4.553498	2.477538	1.375411
24	1	0	2.434679	1.293350	0.917114
25	17	0	-0.048456	-1.144604	1.875574
26	1	0	-2.326025	-2.440731	0.683477
27	1	0	-2.646798	2.525878	-0.139908
28	17	0	-5.124817	1.293596	-0.879891

Zero-point correction= 0.184869 (Hartree/Particle)
Thermal correction to Energy= 0.202443

Thermal correction to Enthalpy=	0.203387
Thermal correction to Gibbs Free Energy=	0.136940
Sum of electronic and zero-point Energies=	-1776.087412
Sum of electronic and thermal Energies=	-1776.069838
Sum of electronic and thermal Enthalpies=	-1776.068894
Sum of electronic and thermal Free Energies=	-1776.135340

$IN_1(P_1)$ in Fig. 4B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.888203	-1.371548	0.163306
2	6	0	3.750853	-0.428477	-0.258076
3	6	0	3.413218	1.042751	-0.183942
4	6	0	2.076505	1.390108	0.335058
5	6	0	1.208902	0.444470	0.738791
6	6	0	1.580401	-1.009983	0.747230
7	8	0	0.848980	-1.855684	1.248701
8	8	0	4.200404	1.898157	-0.555258
9	8	0	0.024397	0.817409	1.310661
10	7	0	-1.079011	0.111637	0.778318
11	6	0	-2.033135	0.929117	0.167105
12	8	0	-1.806615	2.086357	-0.140806
13	6	0	-3.328895	0.230999	-0.122956
14	6	0	-4.459212	1.036451	-0.326220
15	6	0	-5.695730	0.452432	-0.596974
16	6	0	-5.811800	-0.939147	-0.677087
17	6	0	-4.685771	-1.745631	-0.490372
18	6	0	-3.446330	-1.165549	-0.213381
19	1	0	-1.377680	-0.596564	1.440094
20	1	0	-4.347396	2.114117	-0.271069
21	1	0	-6.568007	1.081336	-0.747772
22	1	0	-6.774832	-1.393161	-0.891627
23	1	0	-4.769053	-2.825405	-0.569153
24	1	0	-2.573034	-1.801570	-0.103614
25	17	0	5.302730	-0.831655	-0.905767
26	1	0	3.120045	-2.430528	0.127942
27	1	0	1.816047	2.442576	0.363736

Zero-point correction=	0.186726 (Hartree/Particle)
Thermal correction to Energy=	0.202970
Thermal correction to Enthalpy=	0.203914
Thermal correction to Gibbs Free Energy=	0.139695
Sum of electronic and zero-point Energies=	-1315.812782
Sum of electronic and thermal Energies=	-1315.796538
Sum of electronic and thermal Enthalpies=	-1315.795594
Sum of electronic and thermal Free Energies=	-1315.859813

TS_{1a} in Fig. 4B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.736135	-1.947357	0.349696
2	6	0	-4.030078	-1.612492	0.509520
3	6	0	-4.611106	-0.372063	-0.109924
4	6	0	-3.671578	0.480936	-0.843019
5	6	0	-2.366505	0.162062	-1.007638
6	6	0	-1.825594	-1.130739	-0.480753
7	8	0	-0.698257	-1.546380	-0.746302
8	8	0	-5.802464	-0.093642	0.009389
9	8	0	-1.562808	0.948453	-1.770094
10	7	0	-0.443999	1.437682	-0.999029
11	6	0	-0.714420	2.639671	-0.401418
12	8	0	-1.844108	3.136200	-0.331412
13	6	0	0.469246	3.308840	0.263825
14	6	0	0.176096	4.364669	1.141979
15	6	0	1.200453	5.043804	1.801143
16	6	0	2.534241	4.677748	1.585796
17	6	0	2.831547	3.633593	0.706496
18	6	0	1.808525	2.948344	0.044246
19	1	0	0.519372	1.099240	-1.498064
20	1	0	-0.864446	4.635497	1.287422
21	1	0	0.959605	5.857232	2.481366
22	1	0	3.334850	5.205002	2.099387
23	1	0	3.860782	3.337144	0.525605
24	1	0	2.072866	2.152587	-0.648160
25	17	0	-5.117319	-2.609056	1.440578
26	1	0	-2.310374	-2.847302	0.780129

27	1	0	-4.053433	1.415837	-1.236071
28	8	0	1.679665	0.613515	-2.101306
29	7	0	2.010080	-0.512094	-1.434513
30	6	0	3.220938	-0.702068	-0.858723
31	8	0	4.138026	0.135229	-0.859221
32	6	0	3.403717	-2.047062	-0.193371
33	6	0	4.395823	-2.141225	0.795505
34	6	0	4.636762	-3.346750	1.454884
35	6	0	3.896101	-4.488052	1.128667
36	6	0	2.917489	-4.409917	0.133445
37	6	0	2.674930	-3.201563	-0.525047
38	1	0	1.238830	-1.150430	-1.261129
39	1	0	4.969769	-1.248617	1.021903
40	1	0	5.404729	-3.397763	2.222903
41	1	0	4.084624	-5.429458	1.638499
42	1	0	2.345627	-5.293309	-0.139229
43	1	0	1.925915	-3.170081	-1.309872

Zero-point correction= 0.302040 (Hartree/Particle)
Thermal correction to Energy= 0.327639
Thermal correction to Enthalpy= 0.328584
Thermal correction to Gibbs Free Energy= 0.240346
Sum of electronic and zero-point Energies= -1791.329888
Sum of electronic and thermal Energies= -1791.304288
Sum of electronic and thermal Enthalpies= -1791.303344
Sum of electronic and thermal Free Energies= -1791.391581

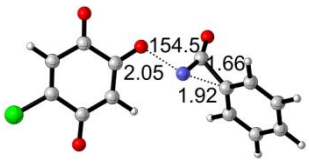
IN_2 in Fig. 4B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.688171	1.050268	0.000127
2	6	0	-3.895707	-0.276611	0.000019
3	6	0	-2.761815	-1.281374	-0.000108
4	6	0	-1.432179	-0.728434	-0.000203
5	6	0	-1.189089	0.626005	-0.000057
6	6	0	-2.318365	1.615280	0.000069
7	8	0	-2.154789	2.831028	0.000120
8	8	0	-3.012204	-2.493238	-0.000133

9	8	0	-0.004672	1.205796	-0.000044
10	7	0	1.089069	0.294230	-0.000050
11	6	0	2.233200	1.014674	-0.000037
12	8	0	2.389523	2.250413	-0.000064
13	6	0	3.453843	0.104251	-0.000006
14	6	0	4.716777	0.712811	-0.000103
15	6	0	5.882555	-0.057054	-0.000057
16	6	0	5.802846	-1.453256	0.000088
17	6	0	4.546223	-2.069689	0.000180
18	6	0	3.381346	-1.298682	0.000135
19	1	0	4.750786	1.797749	-0.000208
20	1	0	6.854025	0.432391	-0.000131
21	1	0	6.708565	-2.055344	0.000131
22	1	0	4.473112	-3.154875	0.000297
23	1	0	2.406903	-1.773599	0.000201
24	17	0	-5.520387	-0.926863	0.000047
25	1	0	-4.498584	1.771208	0.000224
26	1	0	-0.603362	-1.421601	-0.000282

Zero-point correction= 0.172915 (Hartree/Particle)
Thermal correction to Energy= 0.188947
Thermal correction to Enthalpy= 0.189891
Thermal correction to Gibbs Free Energy= 0.125595
Sum of electronic and zero-point Energies= -1315.313781
Sum of electronic and thermal Energies= -1315.297749
Sum of electronic and thermal Enthalpies= -1315.296805
Sum of electronic and thermal Free Energies= -1315.361100

TS_2 in Fig. 4B1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.528502	0.596855	0.116615
2	6	0	2.344943	1.273656	-0.583472
3	8	0	2.666904	2.192542	-1.314555

4	6	0	3.377231	0.090653	-0.056399
5	8	0	-0.231960	1.640179	0.009544
6	6	0	-1.269581	0.911765	0.033022
7	6	0	3.655898	-0.990086	-0.902125
8	6	0	4.774720	-1.788605	-0.658347
9	6	0	5.606798	-1.518209	0.434341
10	6	0	5.315142	-0.446547	1.286643
11	6	0	4.197096	0.354200	1.047786
12	6	0	-1.330687	-0.479508	-0.073045
13	6	0	-2.536628	-1.241887	-0.067513
14	6	0	-3.829484	-0.445459	0.070322
15	6	0	-3.858597	0.890313	0.189913
16	6	0	-2.601239	1.674373	0.200450
17	8	0	-2.603950	-2.478255	-0.168718
18	8	0	-2.643241	2.889230	0.342167
19	1	0	2.995663	-1.196935	-1.738753
20	1	0	4.992390	-2.627887	-1.313870
21	1	0	6.473213	-2.145643	0.626234
22	1	0	5.953851	-0.242347	2.142262
23	1	0	3.951330	1.180071	1.708313
24	17	0	-5.320998	-1.366141	0.068274
25	1	0	-0.404025	-1.032006	-0.169438
26	1	0	-4.780663	1.453622	0.291325

Zero-point correction= 0.168526 (Hartree/Particle)
Thermal correction to Energy= 0.185442
Thermal correction to Enthalpy= 0.186386
Thermal correction to Gibbs Free Energy= 0.118610
Sum of electronic and zero-point Energies= -1315.277579
Sum of electronic and thermal Energies= -1315.260663
Sum of electronic and thermal Enthalpies= -1315.259719
Sum of electronic and thermal Free Energies= -1315.327496

CBQO^{-} in Fig. 4B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.948861	-0.304858	0.000057
2	6	0	0.767791	1.494830	-0.000032

3	6	0	1.825762	0.553536	-0.000047
4	6	0	-0.026340	-1.280824	0.000112
5	1	0	1.029807	2.548974	-0.000166
6	1	0	-0.285469	-2.335157	0.000054
7	8	0	3.045695	0.817386	-0.000123
8	17	0	-2.657541	-0.720086	-0.000101
9	6	0	1.416922	-0.946345	0.000311
10	8	0	2.248458	-1.847537	-0.000098
11	6	0	-0.614357	1.185492	0.000108
12	8	0	-1.555608	2.007233	0.000068

Zero-point correction=	0.066555 (Hartree/Particle)
Thermal correction to Energy=	0.074882
Thermal correction to Enthalpy=	0.075826
Thermal correction to Gibbs Free Energy=	0.032229
Sum of electronic and zero-point Energies=	-915.713771
Sum of electronic and thermal Energies=	-915.705445
Sum of electronic and thermal Enthalpies=	-915.704500
Sum of electronic and thermal Free Energies=	-915.748097

TS_2 in Fig. 4B2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.093215	2.408011	-0.336693
2	6	0	-1.184721	2.018597	0.064573
3	6	0	-1.382833	0.925710	1.069953
4	6	0	-0.212147	0.098010	1.325966
5	6	0	1.010445	0.427959	0.842484
6	6	0	1.232068	1.639588	-0.022025
7	8	0	2.408827	1.946096	-0.396608
8	8	0	-2.479709	0.719805	1.598319
9	8	0	2.059024	-0.336900	1.282712
10	7	0	3.202981	-0.311264	0.449057
11	6	0	4.271823	-0.997714	0.941489
12	8	0	4.249593	-1.721366	1.936071
13	6	0	5.521327	-0.832565	0.105133
14	6	0	6.720193	-1.311297	0.651872
15	6	0	7.918371	-1.191387	-0.052876

16	6	0	7.931588	-0.594490	-1.317658
17	6	0	6.738581	-0.121680	-1.871966
18	6	0	5.538231	-0.240176	-1.167625
19	1	0	6.683421	-1.777136	1.631124
20	1	0	8.841461	-1.563832	0.383643
21	1	0	8.863696	-0.501594	-1.868965
22	1	0	6.738387	0.336650	-2.857077
23	1	0	4.619732	0.118720	-1.620332
24	17	0	-2.451621	3.262984	0.027712
25	8	0	-1.859631	0.846247	-1.341809
26	7	0	-3.087924	0.370169	-1.142978
27	6	0	-3.353725	-0.933050	-0.802839
28	8	0	-2.522075	-1.837539	-0.835649
29	6	0	-4.802508	-1.186671	-0.467709
30	6	0	-5.389195	-2.378015	-0.918462
31	6	0	-6.721711	-2.665841	-0.622258
32	6	0	-7.479261	-1.772859	0.144403
33	6	0	-6.891780	-0.597174	0.619689
34	6	0	-5.558918	-0.303043	0.317423
35	1	0	-3.831436	1.061704	-1.118409
36	1	0	-4.781110	-3.069654	-1.493236
37	1	0	-7.169178	-3.588317	-0.983518
38	1	0	-8.515714	-1.999630	0.381048
39	1	0	-7.465368	0.086106	1.240508
40	1	0	-5.087272	0.582516	0.733421
41	1	0	3.240473	0.633984	-0.009603
42	1	0	0.235354	3.282791	-0.959012
43	1	0	-0.342785	-0.767603	1.965215

Zero-point correction= 0.305127 (Hartree/Particle)
Thermal correction to Energy= 0.330202
Thermal correction to Enthalpy= 0.331147
Thermal correction to Gibbs Free Energy= 0.245443
Sum of electronic and zero-point Energies= -1791.319251
Sum of electronic and thermal Energies= -1791.294176
Sum of electronic and thermal Enthalpies= -1791.293232
Sum of electronic and thermal Free Energies= -1791.378935

$IN_2(P_2)$ in Fig. 4B2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.404535	-1.700008	1.388587
2	6	0	-1.358280	-1.675193	0.438434
3	6	0	-1.019593	-1.767456	-1.028226
4	6	0	0.404708	-1.699485	-1.389211
5	6	0	1.358453	-1.675143	-0.439047
6	6	0	1.019760	-1.767965	1.027580
7	8	0	1.900950	-1.907922	1.868601
8	8	0	-1.900807	-1.906910	-1.869310
9	8	0	2.671421	-1.742073	-0.807837
10	7	0	3.479084	-0.803288	-0.124869
11	6	0	4.190707	0.049468	-0.970784
12	8	0	3.934212	0.168504	-2.156478
13	6	0	5.254274	0.841567	-0.268529
14	6	0	6.284273	1.373818	-1.058063
15	6	0	7.304010	2.119682	-0.468728
16	6	0	7.298067	2.348939	0.911109
17	6	0	6.266186	1.833461	1.700106
18	6	0	5.245985	1.080584	1.115269
19	1	0	3.955991	-1.260807	0.644830
20	1	0	6.265863	1.195288	-2.127971
21	1	0	8.101669	2.524274	-1.084548
22	1	0	8.090928	2.933408	1.368720
23	1	0	6.248851	2.024654	2.768829
24	1	0	4.432637	0.713402	1.733925
25	8	0	-2.671243	-1.742170	0.807208
26	7	0	-3.478889	-0.803116	0.124579
27	1	0	-3.955528	-1.260271	-0.645504
28	6	0	-4.190864	0.049002	0.970848
29	8	0	-3.934696	0.167332	2.156679
30	6	0	-5.254420	0.841336	0.268834
31	6	0	-5.245799	1.081291	-1.114801
32	6	0	-6.284655	1.372975	1.058471
33	6	0	-6.265911	1.834485	-1.699384
34	1	0	-4.432130	0.714810	-1.733449
35	6	0	-7.304346	2.119086	0.469371
36	1	0	-6.266476	1.193770	2.128270
37	6	0	-7.298110	2.349219	-0.910319
38	1	0	-6.248432	2.026240	-2.768004

39	1	0	-8.102236	2.523134	1.085250
40	1	0	-8.090843	2.934029	-1.367714
41	1	0	0.657387	-1.684113	-2.443867
42	1	0	-0.657212	-1.685044	2.443250

Zero-point correction= 0.307413 (Hartree/Particle)
Thermal correction to Energy= 0.331320
Thermal correction to Enthalpy= 0.332265
Thermal correction to Gibbs Free Energy= 0.248319
Sum of electronic and zero-point Energies= -1331.034761
Sum of electronic and thermal Energies= -1331.010853
Sum of electronic and thermal Enthalpies= -1331.009909
Sum of electronic and thermal Free Energies= -1331.093855